

# Detonation failure in stratified layers - the influence of detonation regularity

André Vagner Gaathaug, Knut Vaagsaether and Dag Bjerketvedt  
Univesity College of Southeast Norway  
Porsgrunn, Telemark, Norway

## 1 Introduction

Detonation propagation in stratified fuel layers have been given a new interest recent years, mainly due to the development of hydrogen infrastructure and fuel cell vehicles. An accidental leak of hydrogen could form a fuel layer at the ceiling. The propagation of a detonation in such a layer is important to understand, especially the limits to where the detonation will fail. Recent studies by the KIT group and the University of Warsaw [1, 2] have found a criteria for successful detonation propagation in a layer to be three cell size thick. While more recent studies show that the critical layer thickness varies with the mixtures [3]. Addition of methane to a hydrogen-air mixture increased the critical layer thickness, as shown by Rudy et al. [4]. A study by Houim and Fievisohn [5] investigated the influence of the ratio of sound speed between the reactant and inert layer on the detonation propagation. They showed that a much denser inert or a much lighter inert gas is required to have a successful detonation propagation. They showed numerically how new triple points originate from the interface between inert and reactants. The current study aims to address a similar problem based on a simplified analysis. The authors suggest that detonations with an irregular cellular pattern will propagate further into a stratified layer of reactants compared to a detonation with regular cellular pattern. The highly regular detonation front does not generate any new triple points, and the point will eventually diffract into the inert layer below the fuel layer. A sketch of a suggested failing detonation in a layer of reactants is given in Figure 1. The red arrow illustrate the direction of where the failing detonation as the triple points are "lost" into the inert layer. The earlier work by Sommers [6] also showed the influence on inert gas density on the propagation of detonations. It was discussed how the diffraction gave a lower pressure and temperature, and also how a higher adiabatic index gave a higher post shock pressure and thus a lower velocity deficit. The influence of adiabatic index is not discussed in this work.

## 2 Methods

The method of investigation is computational fluid dynamics using a 2D finite volume method developed by Vaagsaether [7]. It is a explicit method solving the Euler equations with a flux limiting centered scheme.

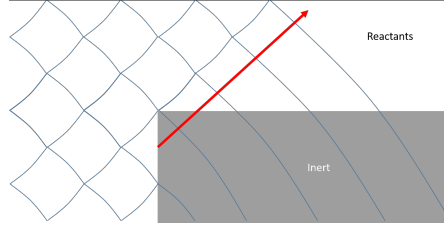


Figure 1: The proposed failure of a stable detonation in a stratified fuel layer. As the triple points are lost into the inert layer, the failure of the detonation will follow the red line.

The method used a two step model for the chemical reactions, where the first is an isothermal reaction in the induction zone. While the second step is the exothermic reactions. The rates are given as:

$$\frac{\partial \alpha}{\partial t} = -A \exp\left(\frac{E_\alpha}{RT}\right) \quad (1)$$

$$\frac{\partial \beta}{\partial t} = B(1 - \beta) \exp\left(\frac{E_\beta}{RT}\right) \mathcal{H}(\alpha - 1) \quad (2)$$

Following this gives an induction time

$$\tau = A \exp\left(\frac{T_\alpha}{T}\right) \quad (3)$$

To narrow the investigation down to the influence of detonation regularity the stability discussion of Austin [8] and Lee and Stewart [9] was taken as a basis. The parameter investigated in the study are the heat of combustion  $q$  and the induction zone reaction activation energy  $E_\alpha$ . The investigation is independent of the numerical resolution as the induction length was set to 10 computational cells, and hence the pre-exponential factor was scaled accordingly to a 1D assumption of the detonation front.

$$(S_{CJ} - u_{vN}) \tau = (S_{CJ} - u_{vN}) A \exp\left(\frac{T_\alpha}{T}\right) = 1 \quad (4)$$

As the size of one numerical cell is set to  $\delta x = \delta y = 0.1$ . The heat capacity ratio was constant for both reactants and inert  $\lambda = 1.4$ . Initial reactant and inert pressure and density was set to  $p = 1$  and  $\rho = 1$ .

Table 1: The numerical input for the pre-exponential factor A.

		A			
q	M	$E_\alpha = 30$	$E_\alpha = 40$	$E_\alpha = 50$	$E_\alpha = 60$
30	6.57	2.773E-02	9.491E-03	3.248E-03	1.111E-03
25	6.02	1.733E-02			

The initial simulations was set as a slightly perturbed planar ZND detonation in a 600 by 2000 domain with an inflow velocity close to the CJ velocity and zero gradient pressure. This was done to reduce the

computational cost. The outflow boundary was set to zero gradient velocity and pressure. The detonation was set to propagate until it gave a stable detonation, in the sense that selected properties of the front did oscillated around stable values. This assumption had to be chosen to make sure all initial detonation fronts were as much as possible independent on the initial conditions. The properties chosen for the evaluation of the development of the detonation front was the x direction induction length. The reaction model was set to give 10 cells in a 1D case. The 2D case is obviously different, but a plot of the x-direction induction length (at one timestep) is given in Figure 2. It shows that it is close to the values of 10 cells in the induction length (based on an ideal 1D assumption). An other property chosen for the development were a plot of the detonation front to investigate the cellular pattern made by the position of the reaction front  $R_{rx}(x, y, t)$ . The reaction front position was adjusted to the mean position of the reaction front. A plot of a reaction front is given in Figure 3. The last parameter to investigate to evaluate the development of the detonation structure was the standard deviation of the reaction front position  $R_{rx}(x, y, t = t_j)$ , shown in Figure 3. This should not be constant for this unsteady system but it oscillates around a near constant value. Based on this, the initial detonation structure was set to be developed.

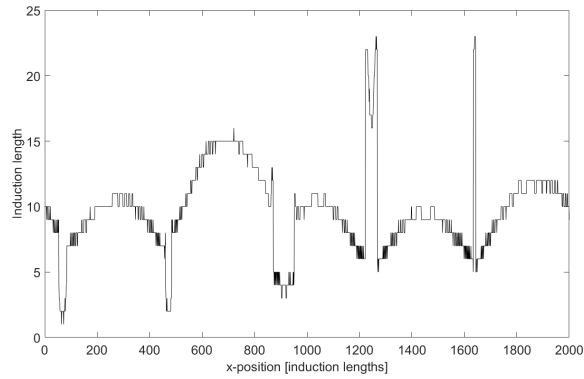


Figure 2: The calculated x-direction induction length.

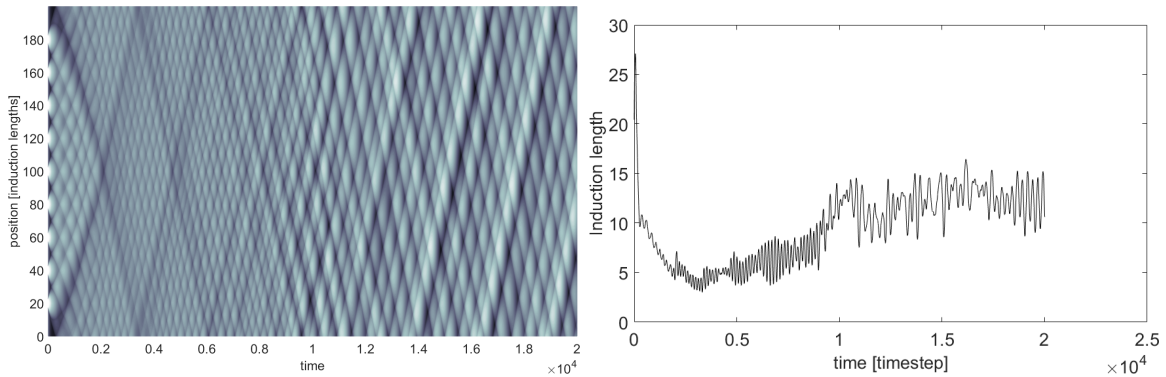


Figure 3: Left: Reaction front position; Right: The standard deviation of the reaction front position.

The setup for the stratified reactant layer was similar to the sketch in Figure 1. The thickness of the reactant layer was chosen to 100 induction lengths, which was less than three detonation cells in most cases. The top boundary was a reflecting wall while the bottom boundary was open zero gradient pressure and velocity. The inert layer was modeled as a convected fuel variable  $f$ , where  $f = 1$  is reactants and  $f = 0$  is inert. There were no diffusion between reactants and inert, except the numerical diffusion.

### 3 Results

The most regular detonation front considered in this work was the  $q = 25$  and  $E_\alpha = 30$ . The sensitivity of the induction reaction to small perturbations is low, and hence it will be harder to generate new triple points as the detonation propagates in the stratified reactant layer. A numerical soot-foil like record were generated from the simulations integrating the pressure in the induction zone. Displaying a scaled gradient of this gives a cellular pattern, similar to soot foil records. The trajectory of the triple point as they diffract into the inert layer can be shown in plots of scaled gradient.

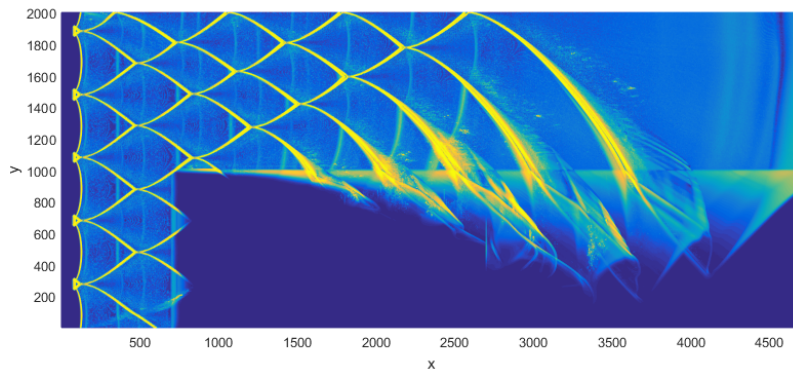


Figure 4: Numerical soot foil for the  $q = 25$  and  $E_\alpha = 30$  case. Showing how the triple points are diffracted into the inert layer. This is considered a reactant mixture with regular cellular detonation pattern.

The failure of the detonation follow the simple idea of triple points diffracting into the inert layer. It does not generate any new triple point, and therefor the detonation fails as the shock and reaction wave decouple. This is seen in Figure 4 where the heat of combustion  $q = 25$  and the induction time activation energy  $E_\alpha = 30$ . As the reactant layer is 100 induction length thick, the detonation fails at a distance of 300 induction lengths into the reactant layer.

By increasing the induction time activation energy (and the heat of combustion from 25 to 30), the regularity of the detonation front changes to more irregular. The reaction becomes more sensitive to small perturbations, and could make new triple point on its own. The results from a more irregular detonation is shown in Figure 7. The case has an heat of combustion  $q = 30$  and an induction time activation energy of  $E_\alpha = 50$ .

It can be seen from the soot foil plot in Figure 7 that the detonation propagates further into the reactant layer as compared to the more regular detonation in Figure 4. The simulations also showed that the mode of propagation changed as the detonation reached the stratified reactant layer. Before the layer, the detonation diffracted into the products. In the layer, the detonation diffracted into the products, but also into the inert layer. This was explained by Sommers in 1961 [6]. A sketch of the explanation is given in Figure 6. It will lead to a velocity deficit of the detonation. An other change in the propagation of the detonation was seen as the propagation before the inert layer was mostly in the axial direction, the transverse direction dominated more when it propagated in the reactant layer. By increasing the thickness of the reactant layer, it is assumed that the detonation will continue further into the reactant layer. A sufficiently thick reactant layer could sustain a detonation as seen in experiments [1, 2, 6].

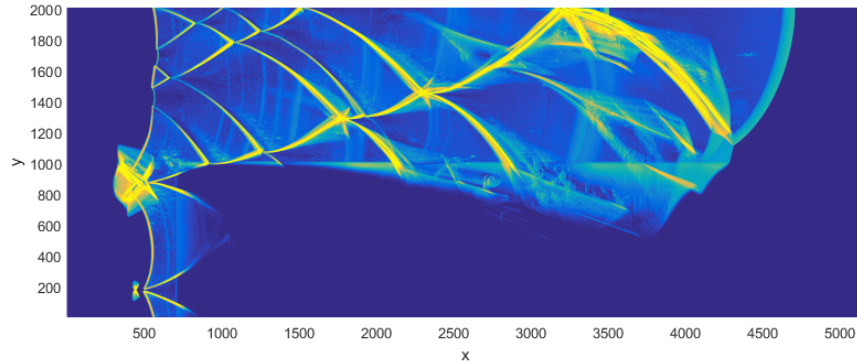


Figure 5: Numerical soot foil for the  $q = 30$  and  $E_\alpha = 50$  case. The triple points are also lost into the inert layer. This reactant mixture results in a larger variance of cell sizes and therefore a more unstable cellular pattern.

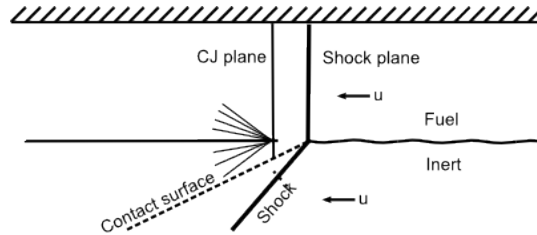


Figure 6:  $H_\alpha$  for the  $q = 25$  and  $E_\alpha = 30$ .

## 4 Further work

This is a beginning of a proposed work on detonations in stratified reactant layers with a focus on single parameters. As this study investigates the influence detonation regularity through activation energy and heat of combustion, there are several other parameters to investigate as well. The influence of the layer thickness is important, as shown in the studies [1, 2]. The aim is to identify if there are limits of layer thickness on the propagation ability. By following the results of Houim and Fievisohn [5], a ratio of speeds of sound should be set and then further investigate the detonation propagation as a function of cellular regularity. At last there will be the influence on adiabatic index,  $\gamma$ , rate of the exothermic reaction, and the influence of species diffusion between reactant and inert layer.

## 5 Summary

Numerical simulations of detonations propagating in a stratified reactant layer above an inert layer has been studied, and the failure of the detonation propagation has been shown. The approach has been to reduce the parameters down to the heat of combustion and the activation energy of the induction time reaction. This will influence the regularity of the detonation as higher activation energy will give more irregular cellular structure of the detonation. The simulations were made independent on numerical resolution as it is scaled to give 10 cells in the induction zone. A developed detonation was used as an initial condition, and a layer of inert was inserted in the computational domain, as seen in Figure 1. The more stable detonations failed

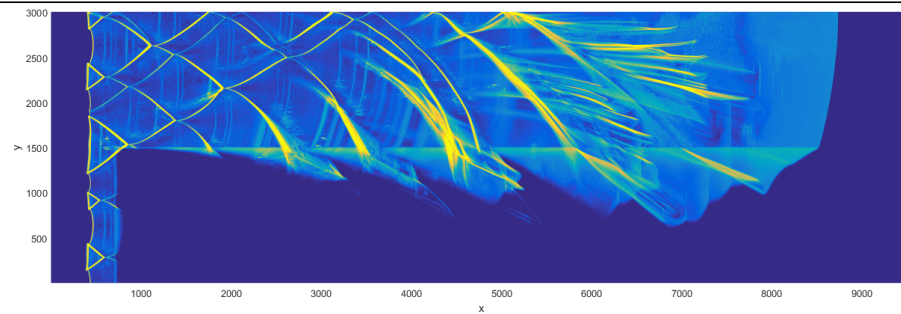


Figure 7: Numerical soot foil for the  $q = 30$  and  $E_\alpha = 50$  case. The triple points are also lost into the inert layer. This reactant mixture results in a larger variance of cell sizes and therefore a more unstable cellular pattern.

as the triple points diffracted into the inert layer, while the more irregular detonations were able to generate new triple points in the reactant layer but eventually failed as well.

## References

- [1] J. Grune, K. Sempert, H. Haberstroh, M. Kuznetsov, and T. Jordan. Experimental investigation of hydrogen–air deflagrations and detonations in semi-confined flat layers. *Journal of Loss Prevention in the Process Industries*, 26(2):317–323, oct 2011.
- [2] W. Rudy, M. Kuznetsov, R. Porowski, a. Teodorczyk, J. Grune, and K. Sempert. Critical conditions of hydrogen-air detonation in partially confined geometry. *Proceedings of the Combustion Institute*, 34(2):1965–1972, jan 2013.
- [3] J Grune, K Sempert, A Friedrich, M Kuznetsov, and T Jordan. ScienceDirect Detonation wave propagation in semi-confined layers of hydrogen e air and hydrogen e oxygen mixtures. *International Journal of Hydrogen Energy*, 42(11):7589–7599, 2016.
- [4] Wojciech Rudy, Mateusz Zbikowski, and Andrzej Teodorczyk. Detonations in hydrogen-methane-air mixtures in semi con fi ned fl at channels. 116:1479–1483, 2016.
- [5] Ryan W Houim and Robert T Fievisohn. The influence of acoustic impedance on gaseous layered detonations bounded by an inert gas. *Combustion and Flame*, 179:185–198, 2017.
- [6] W.P Sommers. *The Interaction of a Detonation Wave with an Inert Boundary*. PhD thesis, 1961.
- [7] K. Vaagsaether. *Modelling of Gas Explosions*. PhD thesis, Telemark University College – NTNU, Norway, 2010.
- [8] J.M. Austin, F. Pintgen, and J.E. Shepherd. Reaction zones in highly unstable detonations. *Proceedings of the Combustion Institute*, 30(2):1849–1857, jan 2005.
- [9] H.I. Lee and D.S. Stewart. Calculation of linear detonation instability : one-dimensional instability of plane detonation. *Journal of fluid mechanics*, 216:103–132, 1990.